[(1-Methylcytosine)2H]I, an asymmetric base pair

Müller, Jens ; Freisinger, Eva

Abstract: The X-ray crystal structure of the title compound, 1-methylcytosinium iodide 1-methylcytosine, [(1-MeC)2H]I (1-MeC is 1-methylcytosine) or C5H8N3O+ · I− · C5H7N3O, has been determined at 163 K. In this compound, one protonated (1-MeCH+) and one neutral methylcytosine (1-MeC) moiety form an asymmetric base pair comprising three hydrogen bonds. A previous structure determination [Krüger, Bruhn Steinborn (2004). Org. Biomol. Chem.2, 2513–2516] showed the same cell parameters but a centrosymmetric base pair in space group P21/c. At low temperature, however, we discovered the title compound to be a racemic twin showing pseudo-centrosymmetry.

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[(1-Methylcytosine)$_2$H]I, an asymmetric base pair

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Key indicators

Single-crystal X-ray study
T = 163 K
Mean σ(C–C) = 0.005 Å
R factor = 0.020
wR factor = 0.043
Data-to-parameter ratio = 13.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The X-ray crystal structure of the title compound, 1-methylcytosinium iodide 1-methylcytosine, [(1-MeC)$_2$H]I (1-MeC is 1-methylcytosine) or $C_5H_8N_3O^+\cdot I^-\cdot C_5H_7N_3O$, has been determined at 163 K. In this compound, one protonated (1-MeCH$^+$) and one neutral methylcytosine (1-MeC) moiety form an asymmetric base pair comprising three hydrogen bonds. A previous structure determination [Krüger, Bruhn & Steinborn (2004). *Org. Biomol. Chem.* **2**, 2513–2516] showed the same cell parameters but a centrosymmetric base pair in space group $P2_1/c$. At low temperature, however, we discovered the title compound to be a racemic twin showing pseudo-centrosymmetry.

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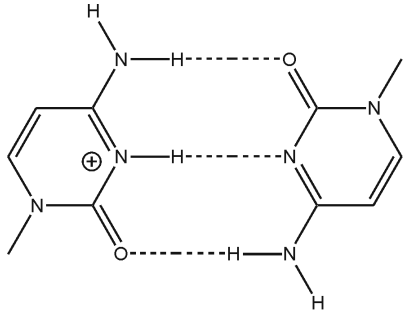
Comment

Hydrogen bonds are a common structural feature in nucleic acids (Lavery & Zakrzewska, 1999). Although typically two different nucleobases undergo base pairing (*e.g.* guanine:cytosine, adenine:thymine), several hydrogen-bonding patterns are known with base pairing between identical nucleobases. The i-motif, consisting of two parallel-stranded intertwined double helices made up entirely of cytosine, is a well known example (Patel *et al.*, 1999). A recent publication describes the crystal structure of a centrosymmetric hemiprotonated methylcytosine:methylcytosine base pair, [(1-MeC)$_2$H]I (Krüger *et al.*, 2004). Concomitant DFT calculations suggest the formation of an asymmetric base pair, however. We report here the crystal structure of this compound in a different crystal configuration, determined at 163 K, displaying the theoretically predicted asymmetric base pairing pattern (Fig. 1). The crystal was obtained in the course of our studies of model systems for metal-mediated base pairs (Müller *et al.*, 2005).



(I)

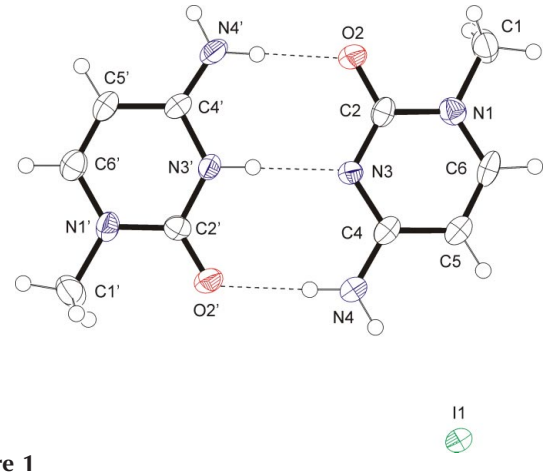


Figure 1
View of the cation of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

The hydrogen-bonded nucleobases of the title compound are almost coplanar [1.6 (2)°]. Two base pairs are bridged *via* the iodide counter-ion (Fig. 2), which forms hydrogen bonds to the exocyclic amine groups of both bases [3.633 (2) and 3.717 (3) Å]. Two crystallographically independent 1-MeC moieties of neighbouring base pairs stack at a distance of approximately 3.4 Å, leading to the formation of a chain structure with two individual chains I and II (Fig. 3).

The H atom at the N3 position of 1-MeCH$^+$ was located in difference Fourier maps. The protonation site is further corroborated by an increase in the C2—N3—C4 angle [125.1 (3)° in 1-MeCH$^+$ and 119.6 (2)° in 1-MeC]. In addition, the two N4(H)···O hydrogen bonds display different bond lengths, resulting in a 2.762 (4) Å distance for the stronger bond involving N4(H) of 1-MeCH$^+$ and 2.901 (3) Å for the weaker bond (see Table 2 for hydrogen-bond geometries). Accordingly, both the C4—N4 and the C2—O2 bonds are significantly shorter in 1-MeCH$^+$ than in 1-MeC [1.291 (5) *versus* 1.333 (4) Å and 1.219 (3) *versus* 1.245 (3) Å]. The N3···N3′ distance is 2.808 (4) Å. All these experimental values correlate well with those of the DFT study (Krüger *et al.*, 2004).

A comparison of the two different crystal forms of [(1-MeC)$_2$H]I with related structures of hemiprotonated cytosine dimers containing a variety of other counter-ions or solvent molecules reveals that in almost all cases asymmetric base pairs are observed (Salam & Aoki, 2000; Schimanski *et al.*, 1998; Kistenmacher *et al.*, 1980; Fujinami *et al.*, 1979; Kistenmacher *et al.*, 1979). Only one of the crystallographically independent 1-MeCH$^+$:1-MeC pairs in the structure of cytosine hemitrichloroacetate has been proposed as truly symmetric (Gdaniec *et al.*, 1988), whereas in the other centrosymmetric structures known to date this symmetry appears to be a consequence of a disordered H atom in the central hydrogen bond (Krüger *et al.*, 2004; Gdaniec *et al.*, 1988). The difference between the crystal structure presented in this work and its symmetric counterpart (Krüger *et al.*, 2004) is presumably based on a temperature-dependent change from disorder to order, supporting this assumption.

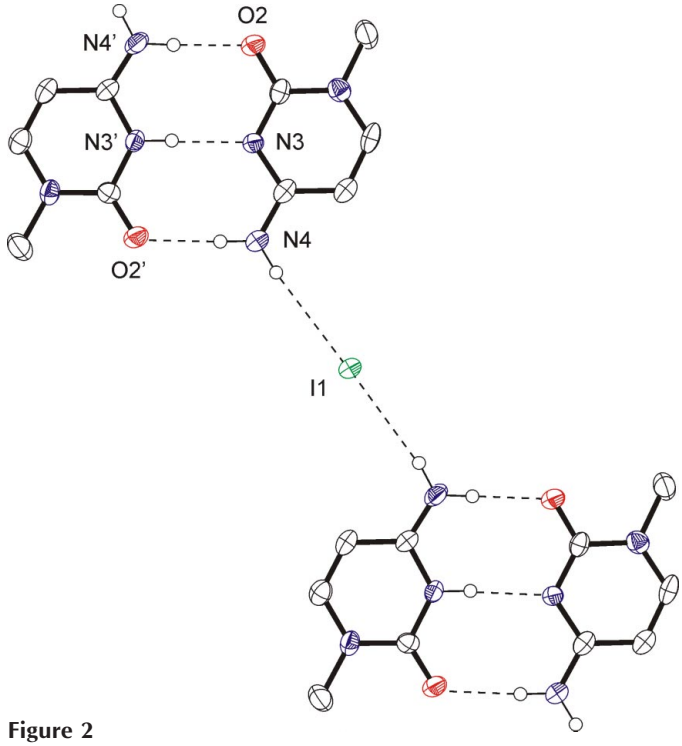


Figure 2
Two base pairs bridged *via* an iodide counter-ion. Displacement ellipsoids are drawn at the 50% probability level. The unlabelled asymmetric pair is related by the symmetry operator ($x+1$, y, $z+1$). Dashed lines indicate hydrogen bonds.

Experimental

The title compound was synthesized according to published protocols (Kistenmacher *et al.*, 1979).

Crystal data

$C_5H_8N_3O^+\cdot I^-\cdot C_5H_7N_3O$
M_r = 378.18
Monoclinic, $P2_1$
a = 7.195 (1) Å
b = 8.629 (2) Å
c = 11.522 (2) Å
β = 97.59 (3)°
V = 709.1 (2) Å^3
Z = 2
D_x = 1.771 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4452 reflections
θ = 2.9–25.4°
μ = 2.27 mm^{-1}
T = 163 (2) K
Block, colourless
0.50 × 0.40 × 0.38 mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.358, T_{max} = 0.427
4462 measured reflections
2519 independent reflections
2291 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 25.4°
$h = -8 \rightarrow 8$
$k = -10 \rightarrow 10$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 4\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.043
S = 0.98
2519 reflections
183 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0118P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0174 (9)
Absolute structure: Flack (1983), 1166 Friedel pairs
Flack parameter: 0.52 (2)

Table 1
Selected geometric parameters (Å, °).

C2—O2	1.245 (3)	C2′—O2′	1.219 (3)
C2—N3	1.359 (4)	C2′—N3′	1.368 (4)
N3—C4	1.342 (3)	N3′—C4′	1.355 (3)
C4—N4	1.333 (4)	C4′—N4′	1.291 (5)
O2—C2—N3	122.3 (3)	O2′—C2′—N3′	121.8 (3)
O2—C2—N1	118.6 (3)	O2′—C2′—N1′	121.7 (4)
N3—C2—N1	119.2 (3)	N3′—C2′—N1′	116.5 (3)
C4—N3—C2	119.6 (2)	C4′—N3′—C2′	125.1 (3)
N4—C4—N3	117.9 (3)	N4′—C4′—N3′	119.7 (3)
N4—C4—C5	119.9 (2)	N4′—C4′—C5′	123.2 (3)
N3—C4—C5	122.2 (3)	N3′—C4′—C5′	117.0 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3′—H3′···N3	0.82 (4)	1.99 (4)	2.808 (4)	171 (4)
N4′—H4′1···O2	0.86	1.92	2.762 (4)	166
N4—H4*A*···O2’	0.86	2.07	2.901 (3)	161
N4—H4*B*···I1	0.86	2.87	3.717 (2)	169
N4′—H4’2···I1^{i}	0.86	2.78	3.633 (2)	171
C5—H5···O2′^{ii}	0.93	2.47	3.088 (4)	124
C5′—H5′···O2^{iii}	0.93	2.48	3.085 (4)	123

Symmetry codes: (i) $x-1, y, z-1$; (ii) $-x+1, y+\frac{1}{2}, -z+1$; (iii) $-x, y-\frac{1}{2}, -z$.

H atoms, except H3′, were included in calculated positions with distances ranging from 0.86 to 0.96 Å and included in the refinement in the riding-model approximation with refined isotropic displacement parameters. Atom H3′ was found in the difference Fourier map and refined without restraints.

Data collection: *KappaCCD Software* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990*b*); software used to prepare material for publication: *SHELXL97*.

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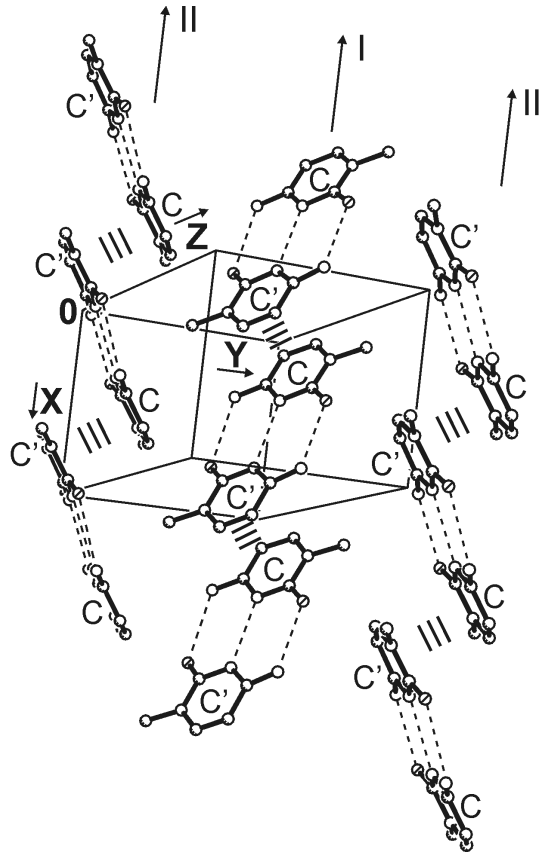

Figure 3
Chain structure formed by base stacking of crystallographically independent 1-MeC moieties. Dashed lines indicate hydrogen bonds.

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supporting information

Acta Cryst. (2005). E**61**, o320–o322 [https://doi.org/10.1107/S1600536805000693]

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$c = 11.522$ (2) Å
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$V = 709.1$ (2) Å^3
$Z = 2$
$F(000) = 372$
$D_x = 1.771$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 4452 reflections
$\theta = 2.9$–25.4°
$\mu = 2.27$ mm^{-1}
$T = 163$ K
Block, colourless
0.50 × 0.40 × 0.38 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 44 pixels mm^{-1}
360 frames via ω–rotation ($\Delta\omega 1°$) and two times 5s per frame scans
Absorption correction: multi-scan (SCALEPACK; Otwinowski & Minor, 1997)
$T_{min} = 0.358$, $T_{max} = 0.427$
4435 measured reflections
2519 independent reflections
2291 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 25.4°$, $\theta_{min} = 2.9°$
$h = -8\rightarrow 8$
$k = -10\rightarrow 10$
$l = -13\rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.020$
$wR(F^2) = 0.043$
$S = 0.98$
2519 reflections
183 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0118P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0174 (9)
Absolute structure: Flack (1983), 1166 Friedel pairs
Absolute structure parameter: 0.52 (2)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Intensity data were collected on an Enraf–Nonius KappaCCD (Nonius BV, Netherlands) (Mo Kα, λ = 0.71069 Å, graphite-monochromator). The structure was solved by standard Patterson methods (Sheldrick 1990*a*) and refined by full-matrix least-squares based on F^2 using the *SHELXTL-Plus* (Sheldrick 1990*b*) and *SHELXL97* (Sheldrick 1997) programs. The positions of all non-hydrogen atoms were deduced from difference Fourier maps and refined anisotropically. Initially, the Flack parameter was refined to a value of 0.51 (2) with: _refine_ls_R_factor_all 0.0263 _refine_ls_R_factor_gt 0.0220 _refine_ls_wR_factor_ref 0.0493 _refine_ls_wR_factor_gt 0.0485 and _refine_ls_goodness_of_fit_ref 1.040 Accordingly, subsequent application of the twin law (-1 0 0, 0 - 1 0, 0 0 - 1) resulted in a racemic twin fraction of 0.51881 with the *R* factors presented below. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
H3′	0.163 (5)	−0.025 (5)	0.248 (3)	0.045 (10)*
I1	0.75919 (2)	0.00071 (13)	0.754516 (15)	0.03646 (9)
N1	0.6507 (4)	0.2149 (4)	0.2055 (4)	0.0297 (9)
C1	0.7037 (5)	0.3110 (5)	0.1102 (3)	0.0419 (10)
H1A	0.7033	0.2488	0.0410	0.048 (4)*
H1B	0.8270	0.3526	0.1325	0.048 (4)*
H1C	0.6157	0.3943	0.0946	0.048 (4)*
C2	0.4866 (4)	0.1298 (4)	0.1845 (3)	0.0261 (8)
O2	0.3983 (3)	0.1308 (3)	0.08405 (16)	0.0308 (6)
N3	0.4287 (3)	0.0467 (3)	0.27326 (19)	0.0230 (8)
C4	0.5352 (4)	0.0432 (4)	0.3781 (3)	0.0252 (10)
N4	0.4765 (3)	−0.0428 (3)	0.4622 (2)	0.0305 (9)
H4A	0.3733	−0.0939	0.4484	0.046 (5)*
H4B	0.5418	−0.0472	0.5302	0.046 (5)*
C5	0.7054 (4)	0.1272 (4)	0.4009 (3)	0.0313 (9)
H5	0.7789	0.1239	0.4736	0.041 (4)*
C6	0.7560 (5)	0.2133 (5)	0.3103 (6)	0.0334 (12)
H6	0.8655	0.2717	0.3218	0.041 (4)*
N1′	−0.1634 (4)	−0.2274 (4)	0.2974 (4)	0.0290 (9)
C1′	−0.2220 (5)	−0.3265 (5)	0.3885 (3)	0.0434 (11)
H1′1	−0.3459	−0.3653	0.3635	0.048 (4)*
H1′2	−0.2223	−0.2677	0.4592	0.048 (4)*
H1′3	−0.1364	−0.4118	0.4028	0.048 (4)*
C2′	0.0013 (4)	−0.1463 (4)	0.3218 (3)	0.0256 (8)
O2′	0.0890 (3)	−0.1442 (3)	0.41984 (17)	0.0319 (6)
N3′	0.0596 (4)	−0.0656 (3)	0.2310 (2)	0.0257 (8)
C4′	−0.0342 (4)	−0.0578 (4)	0.1211 (3)	0.0263 (10)
N4′	0.0347 (3)	0.0217 (6)	0.04203 (19)	0.0351 (8)
H4′1	0.1396	0.0694	0.0592	0.046 (5)*

H4′2	−0.0244	0.0269	−0.0278	0.046 (5)*
C5′	−0.2075 (4)	−0.1396 (4)	0.0995 (3)	0.0303 (9)
H5′	−0.2800	−0.1352	0.0265	0.041 (4)*
C6′	−0.2631 (5)	−0.2221 (5)	0.1857 (5)	0.0316 (12)
H6′	−0.3736	−0.2789	0.1707	0.041 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.03211 (11)	0.04901 (13)	0.02584 (11)	−0.00791 (16)	−0.00519 (7)	0.00848 (13)
N1	0.0295 (16)	0.0269 (18)	0.0332 (19)	0.0005 (16)	0.006 (2)	0.0043 (18)
C1	0.0320 (16)	0.041 (2)	0.053 (2)	−0.0079 (16)	0.0045 (18)	0.010 (2)
C2	0.0184 (13)	0.0252 (19)	0.0337 (18)	0.0049 (13)	0.0000 (15)	−0.0023 (16)
O2	0.0299 (10)	0.0366 (14)	0.0247 (11)	0.0012 (10)	−0.0008 (10)	0.0042 (11)
N3	0.0246 (11)	0.023 (2)	0.0211 (11)	0.0006 (10)	0.0016 (10)	0.0003 (11)
C4	0.0220 (13)	0.026 (3)	0.0269 (15)	0.0071 (12)	−0.0003 (14)	−0.0073 (15)
N4	0.0298 (12)	0.036 (2)	0.0244 (13)	−0.0013 (12)	−0.0026 (12)	0.0021 (14)
C5	0.0274 (15)	0.035 (2)	0.0298 (17)	0.0036 (15)	−0.0040 (15)	−0.0060 (18)
C6	0.018 (2)	0.029 (2)	0.049 (3)	0.0022 (19)	−0.008 (2)	−0.011 (2)
N1′	0.0204 (15)	0.0280 (19)	0.0368 (19)	−0.0002 (16)	−0.0030 (18)	−0.0009 (18)
C1′	0.0327 (17)	0.047 (3)	0.052 (2)	−0.0041 (16)	0.0094 (18)	0.015 (2)
C2′	0.0262 (15)	0.0226 (19)	0.0279 (17)	0.0063 (13)	0.0032 (15)	0.0038 (16)
O2′	0.0305 (10)	0.0371 (15)	0.0264 (11)	0.0023 (10)	−0.0022 (10)	0.0046 (11)
N3′	0.0206 (11)	0.0295 (19)	0.0256 (14)	−0.0020 (11)	−0.0017 (12)	−0.0023 (12)
C4′	0.0258 (14)	0.028 (3)	0.0232 (16)	0.0053 (13)	−0.0024 (15)	−0.0042 (16)
N4′	0.0292 (11)	0.052 (2)	0.0220 (12)	−0.0027 (18)	−0.0041 (11)	−0.004 (2)
C5′	0.0224 (14)	0.034 (2)	0.0318 (18)	0.0028 (14)	−0.0043 (15)	−0.0063 (18)
C6′	0.031 (2)	0.026 (2)	0.036 (3)	0.0009 (19)	−0.001 (2)	−0.005 (2)

Geometric parameters (Å, º)

N1—C6	1.338 (9)	C5′—C6′	1.326 (6)
N1—C2	1.384 (5)	C1—H1A	0.9600
N1—C1	1.466 (5)	C1—H1B	0.9600
C2—O2	1.245 (3)	C1—H1C	0.9600
C2—N3	1.359 (4)	N4—H4B	0.8600
N3—C4	1.342 (3)	N4—H4A	0.8600
C4—N4	1.333 (4)	C5—H5	0.9300
C4—C5	1.417 (4)	C6—H6	0.9300
C5—C6	1.370 (7)	C1′—H1′3	0.9600
N1′—C2′	1.373 (4)	C1′—H1′2	0.9600
N1′—C6′	1.389 (9)	C1′—H1′1	0.9600
N1′—C1′	1.459 (6)	N3′—H3′	0.82 (4)
C2′—O2′	1.219 (3)	N4′—H4′2	0.8600
C2′—N3′	1.368 (4)	N4′—H4′1	0.8600
N3′—C4′	1.355 (3)	C5′—H5′	0.9300
C4′—N4′	1.291 (5)	C6′—H6′	0.9300
C4′—C5′	1.426 (4)		

C6—N1—C2	121.4 (4)	H1′1—C1′—H1′3	109.00
C6—N1—C1	120.6 (3)	H1′2—C1′—H1′3	109.00
C2—N1—C1	118.0 (3)	C2′—N3′—H3′	113 (2)
O2—C2—N3	122.3 (3)	C4′—C5′—H5′	121.00
O2—C2—N1	118.6 (3)	C4′—N3′—H3′	122 (2)
N3—C2—N1	119.2 (3)	C6′—C5′—H5′	121.00
C4—N3—C2	119.6 (2)	C4′—N4′—H4′1	120.00
N4—C4—N3	117.9 (3)	C5′—C6′—H6′	119.00
N4—C4—C5	119.9 (2)	C4′—N4′—H4′2	120.00
N3—C4—C5	122.2 (3)	N1′—C6′—H6′	119.00
C6—C5—C4	116.5 (3)	H4′1—N4′—H4′2	120.00
N1—C6—C5	121.2 (3)	H4A—N4—H4B	120.00
C2′—N1′—C6′	120.0 (4)	C4—N4—H4B	120.00
C2′—N1′—C1′	118.4 (3)	C4—N4—H4A	120.00
C6′—N1′—C1′	121.5 (3)	N1—C1—H1A	109.00
O2′—C2′—N3′	121.8 (3)	N1—C1—H1B	109.00
O2′—C2′—N1′	121.7 (4)	N1—C1—H1C	109.00
N3′—C2′—N1′	116.5 (3)	H1A—C1—H1B	109.00
C4′—N3′—C2′	125.1 (3)	H1A—C1—H1C	109.00
N4′—C4′—N3′	119.7 (3)	H1B—C1—H1C	109.00
N4′—C4′—C5′	123.2 (3)	C4—C5—H5	122.00
N3′—C4′—C5′	117.0 (3)	C6—C5—H5	122.00
C6′—C5′—C4′	118.6 (3)	N1′—C1′—H1′1	109.00
C5′—C6′—N1′	122.8 (3)	N1—C6—H6	119.00
N1′—C1′—H1′3	109.00	N1′—C1′—H1′2	110.00
H1′1—C1′—H1′2	109.00	C5—C6—H6	119.00

C6—N1—C2—O2	−177.1 (3)	C6′—N1′—C2′—O2′	177.5 (3)
C1—N1—C2—O2	4.6 (5)	C1′—N1′—C2′—O2′	−6.9 (5)
C6—N1—C2—N3	2.0 (5)	C6′—N1′—C2′—N3′	−1.2 (5)
C1—N1—C2—N3	−176.4 (3)	C1′—N1′—C2′—N3′	174.4 (3)
O2—C2—N3—C4	176.3 (3)	O2′—C2′—N3′—C4′	−177.4 (3)
N1—C2—N3—C4	−2.7 (4)	N1′—C2′—N3′—C4′	1.3 (5)
C2—N3—C4—N4	−178.3 (3)	C2′—N3′—C4′—N4′	−179.8 (4)
C2—N3—C4—C5	1.6 (4)	C2′—N3′—C4′—C5′	0.5 (5)
N4—C4—C5—C6	−179.8 (3)	N4′—C4′—C5′—C6′	177.8 (4)
N3—C4—C5—C6	0.3 (5)	N3′—C4′—C5′—C6′	−2.4 (5)
C2—N1—C6—C5	0.0 (6)	C4′—C5′—C6′—N1′	2.6 (6)
C1—N1—C6—C5	178.3 (4)	C2′—N1′—C6′—C5′	−0.8 (6)
C4—C5—C6—N1	−1.2 (6)	C1′—N1′—C6′—C5′	−176.2 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3′—H3′···N3	0.82 (4)	1.99 (4)	2.808 (4)	171 (4)
N4′—H4′1···O2	0.86	1.92	2.762 (4)	166
N4—H4*A*···O2′	0.86	2.07	2.901 (3)	161

N4—H4*B*···I1	0.86	2.87	3.717 (2)	169
N4′—H4′2···I1^{i}	0.86	2.78	3.633 (2)	171
C5—H5···O2′^{ii}	0.93	2.47	3.088 (4)	124
C5′—H5′···O2^{iii}	0.93	2.48	3.085 (4)	123

Symmetry codes: (i) $x-1, y, z-1$; (ii) $-x+1, y+1/2, -z+1$; (iii) $-x, y-1/2, -z$.